

3-Methyl-1-nitrobutane
627-67-8 | DTXSID90211769

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 155 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.19e-01

Confidence level: 6.62e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Anisole</div> <div>Measured: 34.7</div> <div>Predicted: 69.5</div>	<div>Image not found</div> <div>para-Xylene</div> <div>Measured: 257</div> <div>Predicted: 246</div>	<div>Image not found</div> <div>p-Cresol</div> <div>Measured: 501</div> <div>Predicted: 95.9</div>
<div>Image not found</div> <div>Toluene</div> <div>Measured: 117</div> <div>Predicted: 87.4</div>	<div>Image not found</div> <div>m-Xylene</div> <div>Measured: 178</div> <div>Predicted: 246</div>	